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Magnetic unmixing of first-order reversal curve diagrams using principal component analysis

Ioan Lascu (1), Richard Harrison (1), Yuting Li (1), Alexander Piotrowski (1), James Channell (2), Joy Muraszko (1), and David Hodell (1)

(1) Department of Earth Sciences, University of Cambridge, Cambridge CB2 3EQ, United Kingdom, (2) Department of Geological Sciences, University of Florida, Gainesville, Florida 32611, United States

We have developed a magnetic unmixing method based on principal component analysis (PCA) of entire first-order reversal curve (FORC) diagrams. FORC diagrams are an advanced hysteresis technique that allows the quantitative characterisation of magnetic grain size, domain state, coercivity and spatial distribution of ensembles of particles within a sample. PCA has been previously applied on extracted central ridges from FORC diagrams of sediment samples containing single domain (SD) magnetite produced by magnetotactic bacteria (Heslop et al., 2014). We extend this methodology to the entire FORC space, which incorporates additional SD signatures, pseudo-single domain (PSD) and multi domain (MD) magnetite signatures, as well as fingerprints of other minerals, such as hematite (HEM). We apply the PCA by resampling the FORC distribution on a regular grid designed to encompass all significant features. Typically 80-90% of the variability within the FORC dataset is described by one or two principal components. Individual FORCs are recast as linear combinations of physically distinct end-member FORCs defined using the principal components and constraints derived from physical modelling.

In a first case study we quantify the spatial variation of end-member components in surficial sediments along the North Atlantic Deep Water (NADW) from Iceland to Newfoundland. The samples have been physically separated into granulometric fractions, which added a further constraint in determining three end members used to model the magnetic ensemble, namely a coarse silt-sized MD component, a fine silt-sized PSD component, and a mixed clay-sized component containing both SD magnetite and hematite (SD+HEM). Sediments from core tops proximal to Iceland are dominated by the SD+HEM component, whereas those closer to Greenland and Canada are increasingly dominated by MD grains. Iceland sediments follow a PSD to SD+HEM trend with increasing grain-size fraction, whereas the Greenland and North America sediments follow a distinct PSD to MD trend. The PCA suggests that fine Icelandic sediments are being transported by NADW flow westward. The presence of the SD+HEM component in all size fractions of the Iceland sediment implies that this fine-grained component is not physically separable from the coarser detrital grains. This is consistent with hematite-coated sediment grains derived from European red sandstones being advected to Iceland. In a second case study we investigate temporal variations of end-member components in binary mixtures from North Atlantic sediment cores collected from the Rockall Basin and the Iberian Margin. Both these locations are characterised by sediments containing magnetosomes and fine detrital PSD grains. For the Rockall Basin samples PCA unmixing was compared to the central ridge extraction quantification method (Egli et al., 2010), yielding quantitatively similar results, whereby the detrital input decreases with time from the Last Glacial Maximum to the Holocene, superimposed on a relatively constant bacterial input. Recent Iberian Margin sediments offer insight into fine-scale variations of detrital PSD and interacting magnetosomes along a redox gradient.